The role of salicylic acid, L-ascorbic acid and oxalic acid in promoting the oxidation of alkenes with H(2)O(2) catalysed by [Mn(IV) (2)(O)(3)(tmtacn)(2)](2+)

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_journal_name_full               'Dalton Trans.'

_journal_coden_Cambridge         0222

_publ_contact_author_name        'Ben Feringa'
_publ_contact_author_email       B.L.FERINGA@RUG.NL

_publ_section_title
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The role of salicylic acid, L-ascorbic acid and oxalic
acid in promoting the oxidation of alkenes with H2O2 catalysed by
[MnIV2(O)3(tmtacn)2]2+
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'Ben Feringa'
'Paul Alsters'
'Wesley Browne'
'Johannes W. de Boer'
'Ronald Hage'
'Auke Meetsma'

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# 0. AUDIT DETAILS

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# 4. TEXT

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_publ_section_abstract
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?
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# Insert blank lines between paragraphs

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The asymmetric unit consists of five moieties:
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a cationic dinuclear Mn-complex, two anionic hexafluoridephosphides
and two disordered, half ethylacetate solvent molecules.
;
_publ_section_exptl_prep
;
?
;
_publ_section_exptl_refinement
;
The structure was solved by Patterson methods and extension of the
model was accomplished by direct methods applied to difference
structure factors using the program DIRDIF.8 The positional and
anisotropic displacement parameters for the non-hydrogen atoms were
refined. Refinement was frustrated by a disorder problem: from the
solution it was clear that the two ethylacetate solvent molecules
were highly disordered, each over an inversion center.
No satisfactory discrete model could be fitted in this density.
The BYPASS procedure was used to squeeze out the disordered
cyclohexane solvent molecule.
Hydrogen atoms were constrained to idealized geometries and
allowed to ride on their carrier atoms with an isotropic
displacement parameter related to the equivalent displacement
parameter of their carrier atoms.

;

Insert blank lines between references

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;
Beurskens, P.T., Beurskens, G., Gelder, R. de Garc\'ia-Granda, S.
Gould, R.O. Isra\"el, & Smits, J.M.M. (1999).
The DIRDIF99 program system, Technical Report of the Crystallography
Laboratory, University of Nijmegen, The Netherlands.

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Spek, A.L. (1990). Acta Cryst. A46, C-34.

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Fig. 1. Chemical structural diagram (scheme 1) of the title compound

Fig. 2. Perspective PLUTO drawing of the molecule illustrating the configuration and the adopted numbering scheme.

Fig. 3. Molecular packing viewed down unit cell axes.

Fig. 4. Perspective ORTEP drawing of the title compound. Displacement ellipsoids for non-H are represented at the 50% probability level.
The H-atoms have been omitted to improve clarity.
;

#==

5. CHEMICAL DATA

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; ?
;
_chemical_name_common   ?
_chemical_melting_point   ?
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Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
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_chemical_formula_sum   'C36 H60 F12 Mn2 N6 O5 P2'
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_chemical_formula_weight   1088.71
_chemical_compound_source   'see text'

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O O 0.0106 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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Mn Mn 0.3368 0.7283 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
F F 0.0171 0.0103 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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6. CRYSTAL DATA

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_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2

loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x,-y,-z

_cell_length_a                   11.4974(5)
_cell_length_b                   13.7430(6)
_cell_length_c                   16.3508(7)
_cell_angle_alpha                76.826(1)
_cell_angle_beta                 76.090(1)
_cell_angle_gamma                69.359(1)
_cell_volume                     2317.49(17)
_cell_formula_units_Z            2

_cell_measurement_temperature    100(1)
_cell_measurement_reflns_used    7227
_cell_measurement_theta_min      2.22
_cell_measurement_theta_max      29.76
_cell_special_details
;
The final unit cell was obtained from the xyz centroids of
7227 reflections after integration using the SAINT software
package (Bruker, 2000).
;

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_exptl_crystal_density_meas      ?
_exptl_crystal_density_diffrn    1.560
_exptl_crystal_density_method    'not measured'
_exptl_crystal_F_000             1124
_exptl_absorpt_coefficient_mu    0.714
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_exptl_absorpt_process_details   '(SADABS, Sheldrick, Bruker, 2001))'
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_diffrn_radiation_detector
;
CCD area-detector
;
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_diffrn_measurement_device_type
;
Bruker Smart Apex
;
_diffrn_measurement_method       'phi and omega scans'
_diffrn_special_details
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Crystal into the cold nitrogen stream of the low-temparature unit
(KRYOFLEX, (Bruker, 2000)).
;
_diffrn_detector_area_resol_mean 66.06

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_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
? ? ?

# number of measured reflections (redundant set)
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_diffrn_reflns_limit_k_min       -17
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_diffrn_reflns_limit_l_min       -21
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_diffrn_reflns_reduction_process
;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to F~o~^2^
using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
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_reflns_number_gt                10023
_reflns_threshold_expression     I>2\s(I)

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_computing_structure_solution
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DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement  'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 2003)
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PLATON (Spek, 1994)
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# 8. REFINEMENT DATA

_refine_special_details
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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F^2^, conventional R-factors R are based
on F, with F set to zero for negative F^2^. The threshold expression of
F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F^2^ are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
;

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_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.0565P)^2^+2.3873P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary   direct
_atom_sites_solution_hydrogens   geom
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_refine_ls_extinction_method     none
_refine_ls_extinction_coef       ?
_refine_ls_abs_structure_details ?
_chemical_absolute_configuration ?

_refine_ls_abs_structure_Flack   ?
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_refine_ls_number_restraints     0
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_refine_ls_R_factor_all          0.0414
_refine_ls_R_factor_gt           0.0384
_refine_ls_wR_factor_ref         0.1078
_refine_ls_wR_factor_gt          0.1052
_refine_ls_goodness_of_fit_ref   1.025
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_refine_ls_shift/su_max          0.001
_refine_ls_shift/su_mean         0.000

_refine_diff_density_max         1.288
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_atom_site_calc_flag
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O13 O Uani 0.37051(12) -0.04199(10) 0.89679(8) 1.000 0.0185(3) . .
O14 O Uani 0.40964(12) 0.13879(10) 0.70930(8) 1.000 0.0194(3) . .
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C16 C Uani 0.14740(18) 0.11458(17) 1.14509(12) 1.000 0.0234(5) . .
C17 C Uani 0.17745(17) 0.11991(15) 1.05697(12) 1.000 0.0193(5) . .
C18 C Uani 0.50325(16) 0.06176(14) 0.68805(10) 1.000 0.0152(4) . .
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C110 C Uani 0.62628(17) 0.18522(15) 0.61458(12) 1.000 0.0205(5) . .
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C132 C Uani 0.21903(18) -0.22329(15) 0.78595(13) 1.000 0.0222(5) . .
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H15 H Uiso 0.19027 0.02308 1.25719 1.000 0.0293 . .
H16 H Uiso 0.08278 0.17067 1.16973 1.000 0.0281 . .
H17 H Uiso 0.13386 0.17999 1.02129 1.000 0.0232 . .
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H117' H Uiso 0.05053 0.41469 0.82796 1.000 0.0239 . .
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H118" H Uiso 0.26332 0.40229 0.79623 1.000 0.0334 . .
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F21 F Uani 0.52540(12) 0.52434(10) 0.20879(8) 1.000 0.0313(4) . .
F22 F Uani 0.31499(13) 0.56320(10) 0.21234(9) 1.000 0.0369(4) . .
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F25 F Uani 0.52620(11) 0.66783(10) 0.10698(8) 1.000 0.0290(4) . .
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F31 F Uani 0.16164(17) 0.26369(15) 0.36068(15) 1.000 0.0679(7) . .
F32 F Uani -0.0266(2) 0.29473(15) 0.44390(10) 1.000 0.0611(7) . .
F33 F Uani 0.00441(19) 0.21713(12) 0.32953(10) 1.000 0.0526(6) . .
F34 F Uani -0.11899(16) 0.38403(15) 0.32836(17) 1.000 0.0723(8) . .
F35 F Uani 0.0746(2) 0.35052(17) 0.24640(11) 1.000 0.0716(7) . .
F36 F Uani 0.03106(14) 0.42926(11) 0.36084(10) 1.000 0.0402(5) . .
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Mn11 0.0137(1) 0.0114(1) 0.0146(1) -0.0025(1) -0.0031(1) -0.0018(1)
Mn12 0.0131(1) 0.0109(1) 0.0142(1) -0.0021(1) -0.0023(1) -0.0025(1)
O11 0.0153(5) 0.0136(6) 0.0181(6) -0.0024(4) -0.0050(4) -0.0025(4)
O12 0.0213(6) 0.0151(6) 0.0161(6) -0.0037(5) -0.0043(5) -0.0018(5)
O13 0.0190(6) 0.0168(6) 0.0180(6) -0.0049(5) -0.0049(5) -0.0012(5)
O14 0.0166(6) 0.0155(6) 0.0240(6) -0.0050(5) 0.0005(5) -0.0042(5)
O15 0.0174(6) 0.0143(6) 0.0209(6) -0.0022(5) 0.0007(5) -0.0032(5)
N11 0.0171(7) 0.0164(7) 0.0223(7) -0.0039(6) -0.0053(6) -0.0030(6)
N12 0.0166(7) 0.0144(7) 0.0197(7) -0.0034(5) -0.0029(5) -0.0028(5)
N13 0.0243(8) 0.0163(7) 0.0200(7) -0.0046(6) -0.0052(6) -0.0019(6)
N14 0.0164(7) 0.0167(7) 0.0205(7) -0.0034(6) -0.0039(5) -0.0035(6)
N15 0.0153(7) 0.0134(7) 0.0187(7) -0.0025(5) -0.0030(5) -0.0039(5)
N16 0.0225(8) 0.0167(7) 0.0181(7) -0.0022(6) -0.0058(6) -0.0039(6)
C11 0.0142(7) 0.0162(8) 0.0167(8) -0.0035(6) -0.0028(6) -0.0058(6)
C12 0.0174(8) 0.0183(8) 0.0154(8) -0.0037(6) -0.0030(6) -0.0074(7)
C13 0.0273(9) 0.0178(9) 0.0208(9) -0.0029(7) -0.0083(7) -0.0067(7)
C14 0.0369(11) 0.0230(9) 0.0205(9) 0.0011(7) -0.0126(8) -0.0134(8)
C15 0.0297(10) 0.0352(11) 0.0158(8) -0.0049(7) -0.0040(7) -0.0184(9)
C16 0.0181(8) 0.0341(11) 0.0219(9) -0.0121(8) -0.0008(7) -0.0099(8)
C17 0.0167(8) 0.0221(9) 0.0195(8) -0.0050(7) -0.0041(6) -0.0049(7)
C18 0.0163(8) 0.0153(8) 0.0135(7) -0.0018(6) -0.0034(6) -0.0041(6)
C19 0.0149(7) 0.0177(8) 0.0144(7) -0.0009(6) -0.0034(6) -0.0048(6)
C110 0.0186(8) 0.0173(8) 0.0242(9) -0.0035(7) -0.0037(7) -0.0040(7)
C111 0.0232(9) 0.0211(9) 0.0339(10) 0.0014(8) -0.0052(8) -0.0111(8)
C112 0.0165(8) 0.0309(10) 0.0267(9) 0.0014(8) -0.0020(7) -0.0094(8)
C113 0.0146(8) 0.0262(10) 0.0231(9) -0.0035(7) -0.0016(7) -0.0022(7)
C114 0.0179(8) 0.0176(8) 0.0173(8) -0.0017(6) -0.0031(6) -0.0040(7)
C115 0.0201(9) 0.0209(9) 0.0316(10) -0.0034(8) -0.0016(7) -0.0078(7)
C116 0.0169(8) 0.0166(8) 0.0232(9) -0.0063(7) -0.0021(6) -0.0014(7)
C117 0.0180(8) 0.0148(8) 0.0237(9) -0.0054(7) -0.0027(7) -0.0003(7)
C118 0.0219(9) 0.0182(9) 0.0293(10) -0.0074(7) -0.0065(7) -0.0058(7)
C119 0.0229(9) 0.0154(8) 0.0226(9) -0.0001(7) -0.0006(7) -0.0040(7)
C120 0.0303(10) 0.0169(9) 0.0202(9) -0.0002(7) -0.0059(7) -0.0016(8)
C121 0.0338(11) 0.0260(10) 0.0195(9) -0.0077(8) -0.0036(8) -0.0019(8)
C122 0.0256(9) 0.0223(9) 0.0274(10) -0.0060(7) -0.0136(8) -0.0015(8)
C123 0.0192(8) 0.0228(9) 0.0290(10) -0.0051(7) -0.0113(7) -0.0019(7)
C124 0.0176(8) 0.0251(10) 0.0277(10) -0.0047(8) 0.0015(7) -0.0053(7)
C125 0.0195(8) 0.0156(8) 0.0209(8) 0.0009(6) -0.0042(6) -0.0058(7)
C126 0.0189(8) 0.0146(8) 0.0180(8) 0.0001(6) -0.0049(6) -0.0036(6)
C127 0.0162(8) 0.0175(8) 0.0290(9) -0.0034(7) -0.0074(7) -0.0037(7)
C128 0.0175(8) 0.0138(8) 0.0236(9) -0.0061(7) -0.0021(7) -0.0012(6)
C129 0.0230(9) 0.0177(8) 0.0216(9) -0.0077(7) -0.0009(7) -0.0027(7)
C130 0.0401(12) 0.0247(10) 0.0191(9) -0.0013(7) -0.0108(8) -0.0068(9)
C131 0.0273(9) 0.0179(9) 0.0266(9) -0.0049(7) -0.0107(7) -0.0071(7)
C132 0.0204(9) 0.0192(9) 0.0297(10) -0.0032(7) -0.0087(7) -0.0071(7)
P21 0.0206(2) 0.0138(2) 0.0245(2) -0.0040(2) -0.0045(2) -0.0031(2)
F21 0.0363(7) 0.0202(6) 0.0365(7) -0.0007(5) -0.0188(5) -0.0021(5)
F22 0.0313(7) 0.0262(7) 0.0473(8) -0.0004(6) 0.0029(6) -0.0117(5)
F23 0.0352(7) 0.0235(6) 0.0343(7) -0.0125(5) -0.0107(5) -0.0045(5)
F24 0.0236(6) 0.0210(6) 0.0416(7) 0.0001(5) -0.0108(5) -0.0018(5)
F25 0.0253(6) 0.0304(7) 0.0342(7) -0.0003(5) -0.0080(5) -0.0133(5)
F26 0.0608(9) 0.0225(6) 0.0294(7) -0.0110(5) -0.0055(6) -0.0068(6)
P31 0.0296(3) 0.0175(2) 0.0232(2) -0.0010(2) -0.0002(2) -0.0006(2)
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```
F31 0.0386(9) 0.0473(10) 0.0944(15) 0.0057(10) -0.0132(9) 0.0052(8)
F32 0.0976(15) 0.0676(12) 0.0303(8) -0.0085(8) 0.0103(8) -0.0544(11)
F33 0.0877(13) 0.0250(7) 0.0419(8) -0.0117(6) -0.0075(8) -0.0126(8)
F34 0.0381(9) 0.0472(10) 0.141(2) -0.0415(12) -0.0419(11) 0.0090(8)
F35 0.0954(16) 0.0689(13) 0.0337(9) 0.0026(8) 0.0066(9) -0.0241(12)
F36 0.0450(8) 0.0242(7) 0.0532(9) 0.0025(6) -0.0187(7) -0.0118(6)

#===============================================================================

# 10. MOLECULAR GEOMETRY

_geom_special_details
;
Bond distances, angles etc. have been calculated using the
rounded fractional coordinates. All su's are estimated
from the variances of the (full) variance-covariance matrix.
The cell esds are taken into account in the estimation of
distances, angles and torsion angles
;

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Mn11 O14 2.0719(15) . . yes
Mn11 N11 2.2442(17) . . yes
Mn11 N12 2.1240(16) . . yes
Mn11 N13 2.2120(17) . . yes
Mn12 O11 1.8173(14) . . yes
Mn12 O13 2.0846(13) . . yes
Mn12 O15 2.0178(14) . . yes
Mn12 N14 2.1975(17) . . yes
Mn12 N15 2.1176(16) . . yes
Mn12 N16 2.2557(16) . . yes
P21 F21 1.6074(15) . . yes
P21 F22 1.6031(16) . . yes
P21 F23 1.6009(14) . . yes
P21 F24 1.6070(15) . . yes
P21 F25 1.5991(15) . . yes
P21 F26 1.5954(14) . . yes
P31 F31 1.620(2) . . yes
P31 F32 1.5824(17) . . yes
P31 F33 1.6029(18) . . yes
P31 F34 1.556(2) . . yes
P31 F35 1.5928(18) . . yes
P31 F36 1.5972(16) . . yes
O12 C11 1.266(2) . . yes
O13 C11 1.255(2) . . yes
O14 C18 1.259(2) . . yes
O15 C18 1.266(2) . . yes
N11 C115 1.476(3) . . yes
N11 C116 1.484(2) . . yes
N11 C123 1.491(3) . . yes
N12 C119 1.498(2) . . yes
N12 C117 1.507(3) . . yes
N12 C118 1.492(3) . . yes
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N13 C121 1.479(3) . . yes
N13 C120 1.496(3) . . yes
N14 C125 1.495(2) . . yes
N14 C132 1.484(3) . . yes
N14 C124 1.479(3) . . yes
N15 C126 1.491(2) . . yes
N15 C127 1.489(3) . . yes
N15 C128 1.505(2) . . yes
N16 C130 1.470(3) . . yes
N16 C131 1.493(3) . . yes
N16 C129 1.483(3) . . yes
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C12 C17 1.399(3) . . no
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C14 C15 1.384(3) . . no
C15 C16 1.386(3) . . no
C16 C17 1.390(3) . . no
C18 C19 1.496(3) . . no
C19 C110 1.388(3) . . no
C19 C114 1.394(3) . . no
C110 C111 1.393(3) . . no
C111 C112 1.385(3) . . no
C112 C113 1.383(3) . . no
C113 C114 1.391(3) . . no
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C14 H14 0.9499 . . no
C15 H15 0.9500 . . no
C16 H16 0.9499 . . no
C116 C117 1.517(3) . . no
C17 H17 0.9500 . . no
C119 C120 1.512(3) . . no
C122 C123 1.521(3) . . no
C125 C126 1.513(3) . . no
C128 C129 1.515(3) . . no
C131 C132 1.524(3) . . no
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C111 H111 0.9500 . . no
C112 H112 0.9500 . . no
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C114 H114 0.9501 . . no
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C126 H126' 0.9900 . . no
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C128 H128 0.9900 . . no
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C129 H129' 0.9900 . . no
C129 H129 0.9899 . . no
C130 H130' 0.9804 . . no
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C130 H130 0.9796 . . no
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C131 H131 0.9900 . . no
C132 H132 0.9900 . . no
C132 H132' 0.9901 . . no

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_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
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O11 Mn11 O14 95.97(6) . . . yes
O11 Mn11 N11 96.73(6) . . . yes
O11 Mn11 N12 175.19(6) . . . yes
O11 Mn11 N13 95.18(6) . . . yes
O12 Mn11 O14 96.78(6) . . . yes
O12 Mn11 N11 88.55(6) . . . yes
O12 Mn11 N12 88.31(6) . . . yes
O12 Mn11 N13 164.69(6) . . . yes
O14 Mn11 N11 165.67(6) . . . yes
O14 Mn11 N12 86.24(6) . . . yes
O14 Mn11 N13 92.80(6) . . . yes
N11 Mn11 N12 80.61(6) . . . yes
N11 Mn11 N13 79.47(6) . . . yes
N12 Mn11 N13 80.41(6) . . . yes
O11 Mn12 O13 95.23(6) . . . yes
O11 Mn12 O15 95.01(6) . . . yes
O11 Mn12 N14 95.43(6) . . . yes
O11 Mn12 N15 175.56(6) . . . yes
O11 Mn12 N16 97.72(6) . . . yes
O13 Mn12 O15 97.34(5) . . . yes
O13 Mn12 N14 93.05(6) . . . yes
O13 Mn12 N15 86.22(6) . . . yes
O13 Mn12 N16 165.63(6) . . . yes
O15 Mn12 N14 164.54(6) . . . yes
O15 Mn12 N15 88.96(6) . . . yes
O15 Mn12 N16 87.76(6) . . . yes
N14 Mn12 N15 80.29(6) . . . yes
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N15 Mn12 N16 80.42(6) . . . yes
F25 P21 F26 90.21(8) . . . yes
F21 P21 F22 90.26(8) . . . yes
F21 P21 F23 89.58(7) . . . yes
F21 P21 F24 179.34(7) . . . yes
F21 P21 F25 90.32(8) . . . yes
F21 P21 F26 90.17(8) . . . yes
F22 P21 F23 89.50(8) . . . yes
F22 P21 F24 89.88(8) . . . yes
F22 P21 F25 179.27(8) . . . yes
F22 P21 F26 90.24(8) . . . yes
F23 P21 F24 89.78(7) . . . yes
F23 P21 F25 90.06(7) . . . yes
F23 P21 F26 179.63(7) . . . yes
F24 P21 F25 89.54(7) . . . yes
F24 P21 F26 90.48(8) . . . yes
F35 P31 F36 89.16(10) . . . yes
F31 P31 F32 87.61(12) . . . yes
F31 P31 F33 91.65(11) . . . yes
F31 P31 F34 178.37(11) . . . yes
F31 P31 F35 87.73(12) . . . yes
F31 P31 F36 88.31(10) . . . yes
F32 P31 F33 90.10(10) . . . yes
F32 P31 F34 93.12(13) . . . yes
F32 P31 F35 175.12(13) . . . yes
F32 P31 F36 89.25(10) . . . yes
F33 P31 F34 89.81(11) . . . yes
F33 P31 F35 91.49(10) . . . yes
F33 P31 F36 179.35(9) . . . yes
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F34 P31 F36 90.24(10) . . . yes
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Mn11 O12 C11 128.43(12) . . . yes
Mn12 O13 C11 129.76(12) . . . yes
Mn11 O14 C18 130.14(13) . . . yes
Mn12 O15 C18 129.11(12) . . . yes
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Mn11 N11 C123 110.00(12) . . . yes
Mn11 N11 C115 111.82(12) . . . yes
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C117 N12 C118 109.37(15) . . . yes
C117 N12 C119 110.23(15) . . . yes
Mn11 N12 C117 111.90(12) . . . yes
Mn11 N12 C118 111.85(12) . . . yes
Mn11 N12 C119 104.93(11) . . . yes
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C120 N13 C122 112.44(17) . . . yes
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Mn11 N13 C120 109.89(12) . . . yes
Mn11 N13 C121 111.92(13) . . . yes
Mn11 N13 C122 103.33(11) . . . yes
C120 N13 C121 109.33(16) . . . yes
C125 N14 C132 112.51(15) . . . yes
Mn12 N14 C132 103.90(11) . . . yes
Mn12 N14 C124 111.30(12) . . . yes
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C124 N14 C132 109.97(16) . . . yes
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C126 N15 C127 109.08(14) . . . yes
Mn12 N15 C128 112.20(11) . . . yes
Mn12 N15 C126 105.41(12) . . . yes
Mn12 N15 C127 110.81(11) . . . yes
C126 N15 C128 110.02(14) . . . yes
C127 N15 C128 109.24(15) . . . yes
C129 N16 C131 112.74(15) . . . yes
Mn12 N16 C129 102.52(12) . . . yes
Mn12 N16 C130 112.84(12) . . . yes
Mn12 N16 C131 109.36(11) . . . yes
C129 N16 C130 109.07(16) . . . yes
C130 N16 C131 110.15(17) . . . yes
O12 C11 C12 116.67(16) . . . yes
O12 C11 O13 124.98(16) . . . yes
O13 C11 C12 118.32(16) . . . yes
C13 C12 C17 119.66(17) . . . no
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C14 C15 C16 120.46(18) . . . no
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O14 C18 O15 124.99(17) . . . yes
O14 C18 C19 117.96(16) . . . yes
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C111 C112 C113 120.4(2) . . . no
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C112 C113 C114 119.91(19) . . . no
C14 C13 H13 120.09 . . . no
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C15 C14 H14 119.90 . . . no
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C15 C16 H16 120.08 . . . no
C17 C16 H16 120.08 . . . no
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C16 C17 H17 119.98 . . . no
N12 C117 C116 111.33(15) . . . yes
C12 C17 H17 119.99 . . . no
N12 C119 C120 110.42(17) . . . yes
N13 C120 C119 109.56(16) . . . yes
N13 C122 C123 111.23(17) . . . yes
N11 C123 C122 110.70(17) . . . yes
N14 C125 C126 109.74(15) . . . yes
N15 C126 C125 110.02(15) . . . yes
N15 C128 C129 111.30(15) . . . yes
N16 C129 C128 110.66(16) . . . yes
N16 C131 C132 110.94(16) . . . yes
N14 C132 C131 111.06(18) . . . yes
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C111 C110 H110 120.11 . . . no
C110 C111 H111 120.00 . . . no
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C113 C112 H112 119.80 . . . no
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H115' C115 H115" 109.48 . . . no
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N11 C116 H116' 109.48 . . . no
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C116 C117 H117 109.37 . . . no
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H118' C118 H118" 109.47 . . . no
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